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Simulation of Rate of Adsorption by Approach of Multiple Regression Model

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Mathematical model was developed to monitor, predict and simulate the rate of adsorption of Crude oil using the approach of multiple regression techniques. The research revealed that the rate of adsorption of crude oil in the process of remediation depends completely on sawdust dosage, weight of adsorbent and concentration of crude oil as well as the independent variables. The functional parameters that controlled the process was monitored and predicted using multiple regression approach in the determination of parameters a_0, a, a_2 and a_3 for the various adsorbent of the wood sawdust A, B, C, and D as presented in this paper. The experimental rate of adsorption was validated with the developed model and the result obtained shows a good match indicating the reliability of the developed model. The research work demonstrates the usefulness of the developed model in monitoring, predicting and simulating the rate of adsorption of wood sawdust of various species in enhancing bioremediation in a polluted site environment.

INTRODUCTION

Crude oil spill is an occurrence that affects the world economically and ecologically. Several materials have been introduced to reduce the effects of crude oil spills; these include synthetic, natural materials-such as agricultural by- products (sawdust, corncob, husk etc) as adsorbent [1-4]. Crude oil is one of the vital energy sources in the world and also a major feedstock for the growing chemical, petrochemical, polymer and other related industries [5 - 6]. In essence, this huge interest in crude oil is the driving force behind our industrial activities today. As long as crude oil is searched for, carried from one place to another, stored and employed for the purpose of refining, there will be the likelihood of a spillage [7]. Oil pollution, as a result of crude oil release on marine environment is now a global concern than other material spilled into the environment. In Nigeria, pollution from spilt oil specifically of the aquatic environment has steadily increased with the increase in oil related activities [8]. In Nigeria, specifically in the Niger Delta area, it is estimated that the total influx of petroleum hydrocarbons spilled over the last five decades is about 1.5 million metric tons [9]. The reason for this spill could be as a result of corrosion, pipeline burst, via willful damage due to illegal refining, means of conveyance, tankers charging and discharging operations, equipment malfunction which may lead to leakages from engines, operators and maintenance error, no prompt maintenance culture, and accidental discharge of industrial oily wastes effluents [10]. Besides, pollution from sources such as flow stations, well heads, drilling site, and offshore oil production area may be attributed to oil spill. Indeed, crude oil pollution on water surroundings, affects life and vegetation [11–15]. The aim of this research is to reduce the harm (ecological and economical) caused by oil spill through bio-adsorption process using local waste material (wood sawdust) as adsorbents for oil spills clean up.

MATERIALS AND METHODS

Materials

Materials and equipment used for the investigation

The material and equipment used in this study are: Adsorbent (sawdust), crude oil, beakers, cylindrical flask, sampling containers(cans), pH meter, electronic balance, reagents, filter paper, funnels, water (fresh and saline), digital water and soil analysis kit, desiccators, oven, sieves mechanical shaker, UV spectrophotometer.

Experimental Methods

Sample Collection and Characterization

The sawdust used for this investigation was collected from a sawmill located in Mile 3 Diobu, Port Harcourt, Rivers State, Nigeria. The fresh water was obtained from the chemical/petrochemical laboratory environment. The Salt water used for this experiment was gotten from the Eagle Island water source Port Harcourt, Rivers State, Nigeria. The various samples (opepe - A, abura - B, mahogany - C, iroko - D) collected were transported to the Department of Chemical/Petrochemical Engineering laboratory for analysis, and determination of the following

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physicochemical parameters: moisture content, pH, porosity, bulk density, kjedahl nitrogen, potassium, phosphorus, carbon and others. Similarly, some of the samples were taken to the Department of Microbiology laboratory for the purpose of isolation, identification and characterization of the possible microorganism present in each sample of the soft, semi hard, and hardwood of small particle size (sawdust).

Crude oil samples were collected from three different oil wells in OML 58 of Total E&P Nigeria limited location in Ogba/Egbema/Ndoni Local Government Area of Rivers State of Niger Delta Area of Nigeria. The various samples collected were taken to the Department of Chemical /Petrochemical Engineering laboratory for physicochemical analysis. The laboratory adsorption experiment was carried out for two water samples (fresh and seawater).

Simulation of Rate of Adsorption (O_a) by Approach of Multiple Regression Model

The rate of adsorption of oil in the process or system of remediation depends completely upon sawdust dosage (X_A), weight of adsorbent (X_B) and concentration of oil waste effluent (X_C) as independent variables. A corresponding linear but multiple regression equation is express in the form:

$$O_a = a_o + a_1 X_A + a_2 X_B + a_3 X_C \qquad (1)$$

Equation (1) is a linear equation of O_a on X_A, X_B and X_C. Because the dependent variable O_a varies partially due to the variations in X_A, X_B and X_C, respectively, the coefficient a_0, a_1, a_2 and a_3 represent partial regression coefficient (coefficient of adsorption rate).

RESULTS AND DISCUSSION

WOOD A: Development of Adsorption Rate for wood A

The generated applicable normal equation is given as;

$$\begin{Bmatrix} 4 & 110 & 28.66 & 560.1 \\ 110 & 3900 & 1001.8 & 3729.1 \\ 28.66 & 1001.8 & 257.57 & 977.6 \end{Bmatrix} \begin{Bmatrix} a_0 \\ a_1 \\ a_2 \end{Bmatrix} = \begin{Bmatrix} 6.66 \\ 221.60 \\ 57.21 \end{Bmatrix} \qquad (2)$$

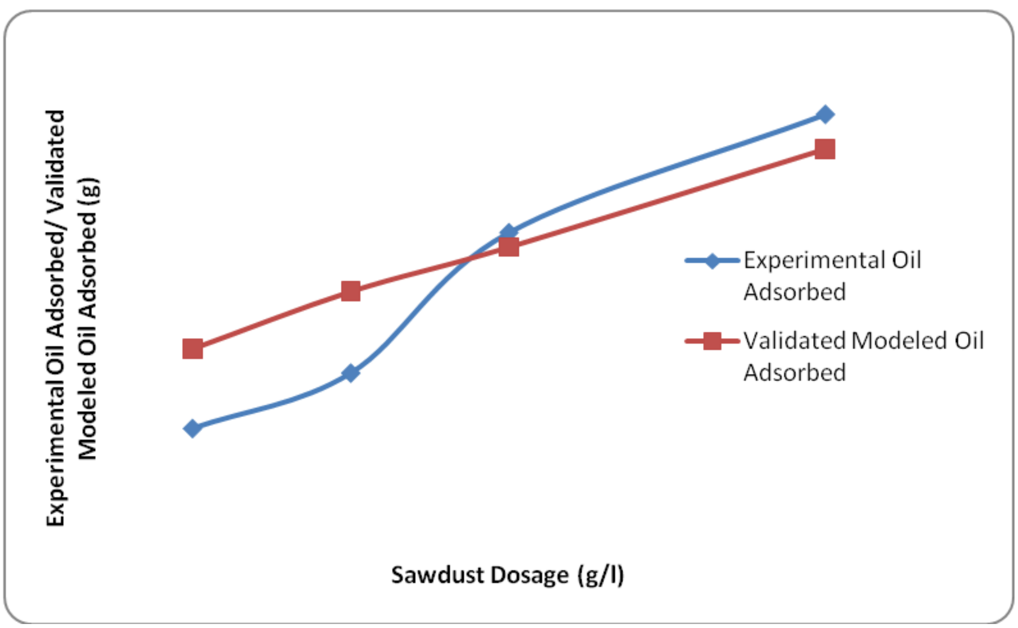

Figure 1 Graph of Experimental oil adsorbed and Validated Modeled oil adsorbed versus Sawdust dosage

Solving Equation (2) using matrix elimination method for solving a set of linear equation gives the below result;

$$\begin{Bmatrix} a_0 \\ a_1 \\ a_2 \end{Bmatrix} - \begin{Bmatrix} 1.0128 \\ 0.0055 \\ 0.0920 \end{Bmatrix} \qquad (3)$$

Substituting the values of Equation (4.3) into Equation (4.1), gives;

$$O_a = 1.0128 + 0.0055X_A + 0.0920X_B - 0.0012X_C \qquad (4)$$

Equation (4) is the Adsorption Rate model for wood type A for the simulation of oil adsorbed during the process of remediation. This equation is a function of sawdust dosage, oil waste effluent and the weight of absorber injected during the process.

The verification of multiple regression model in investigating the adsorption rate of oil pollutant in remediation of a polluted site were assessed by solving the relationship between the experimental oil adsorbed and the modeled oil adsorbed and coefficient of determination of $R^2 = 0.96$ was obtained which indicate the reliability of equation (4) as a valid model. Figure 1 demonstrate the trend behavior between experimental oil adsorbed and modeled oil adsorbed against sawdust which indicate the usefulness of the model tool in predicting the adsorption rate of oil in the process of cleaning a polluted site by applying Wood A. The modeled equation generated is useful in simulating the rate of adsorption oil in the case of Wood A.

Wood B: development of Rate Adsorption (0_a) for wood type B for the purpose of simulation of 0_a

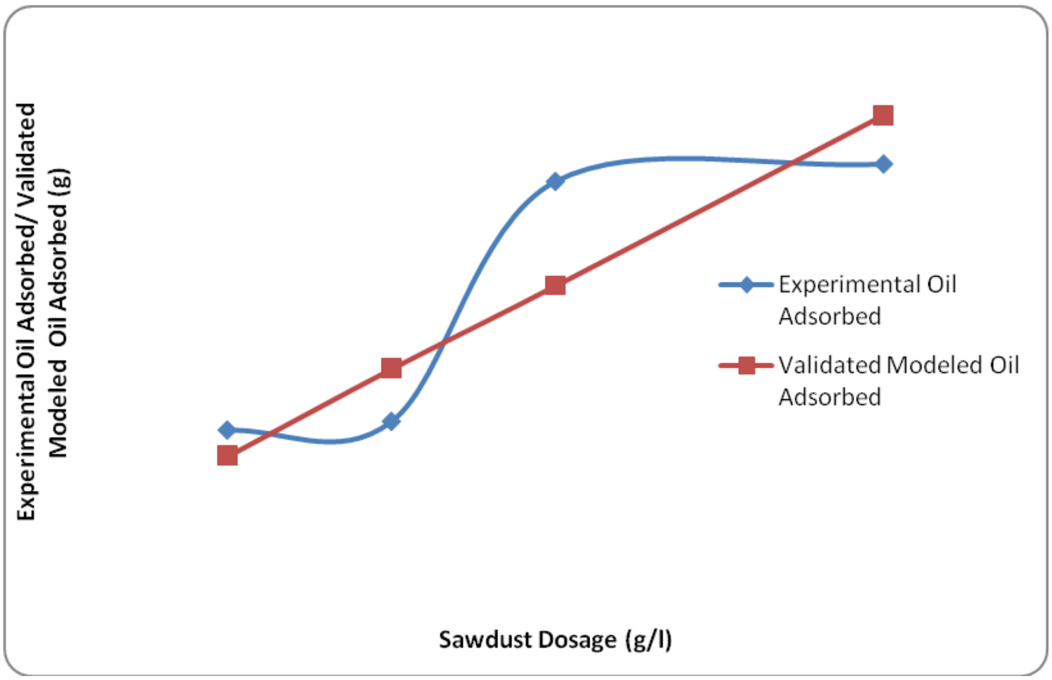

Figure 2 Graph of Experimental oil adsorbed and Validated modeled oil adsorbed versus Sawdust dosage

For this case the applicable normal equation is given as;

$$\begin{Bmatrix} 4 & 110 & 465.5 & 320.5 \\ 110 & 3900 & 825.3 & 8057.5 \\ 465.5 & 825.3 & 196.5 & 1832.9 \\ 320.5 & 8057 & 1832.9 & 26344.5 \end{Bmatrix} \begin{Bmatrix} a_0 \\ a_1 \\ a_2 \end{Bmatrix} = \begin{Bmatrix} 2.9 \\ 95.3 \\ 21.5 \end{Bmatrix}$$

Solving Equation (5) by method of matrix elimination for solving a set of linear equations gives the below result;

$$\begin{Bmatrix} a_0 \\ a_1 \\ a_2 \end{Bmatrix} = \begin{Bmatrix} -0.1050 \\ 0.0216 \\ 0.0001 \end{Bmatrix} \qquad (6)$$

Putting these values into equation (1) yielded;

$$O_a = -0.105 + 0.0216X_A + 0.0001X_B + 0.0028X_C \qquad (7)$$

Equation (7) is the simulation model equation for wood type B for prediction of rate of adsorption of oil in the remediation process. For the aim of the development of this model equation, sawdust, weight of absorbent and contraction of oil waste effluent are the function parameters.

The verification of multiple Regression Model in predicting the Adsorption Rate of oil during remediation in process of a polluted site were determined by shedding the relationship between experimental oil adsorbed and Model oil adsorbed at time of investigation by considering wood B and coefficient of determination $R^2 = 0.76$ were obtained, this validate how good equation (2) is in simulating the adsorption rate in system of remediation and monitoring processes. Figure 2 illustrate the relationship between the experimental results of oil adsorbed obtained in remediation process using Wood B and the validated modeled adsorbed oil by approach of multiple regression model and the trend of behavior as indicated shows acceptability of the developed model in simulating adsorption oil in remediation processes.

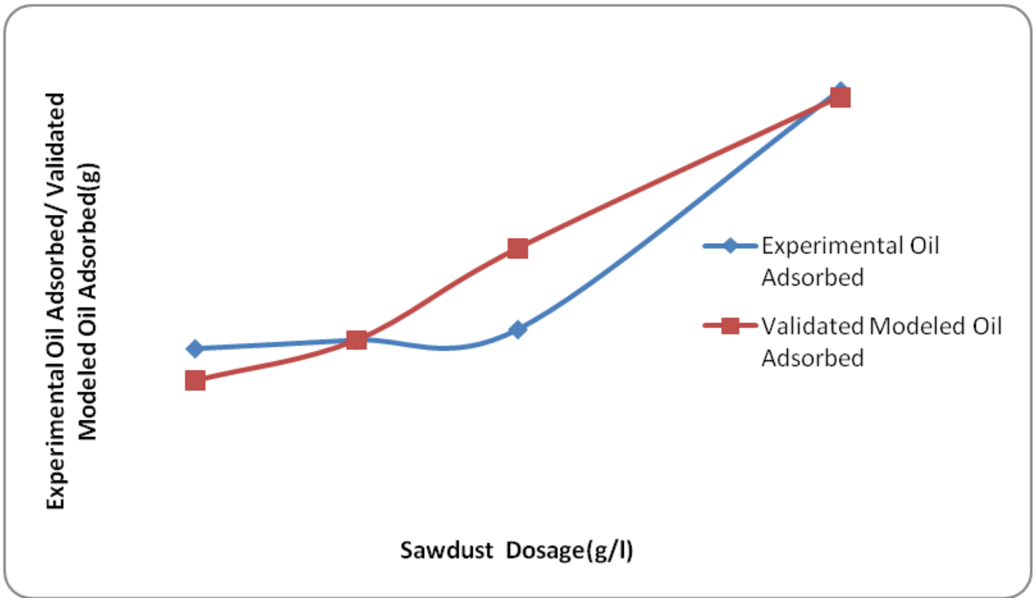

Figure 3 Plot of Experimental oil adsorbed and Validated oil adsorbed against Sawdust dosage

WOOD C: Development of Model equation for wood C that will simulate adsorption rate. The applicable normal equation is of the form;

$$\begin{Bmatrix} 4 & 110 & 32.5 & 116.4 \\ 110 & 3900 & 117.3 & 2850.5 \\ 32.5 & 117.3 & 321.7 & 853.9 \end{Bmatrix} \begin{Bmatrix} a_0 \\ a_1 \\ a_2 \end{Bmatrix} = \begin{Bmatrix} 5.5 \\ 117.3 \\ 51.70 \end{Bmatrix} \qquad (8)$$

Solving Equation (8) by approach of matrix elimination method for solving a set of linear equation gives the result of a_0 a_1 a_2 anda_3 been being the constant coefficient of adsorption rate.

$$\begin{Bmatrix} a_0 \\ a_1 \\ a_2 \end{Bmatrix} = \begin{Bmatrix} 2.0831 \\ 0.0008 \\ 0.0640 \end{Bmatrix} \qquad (9)$$

Putting a_0, a_1, a_2 and a_3 into Equation (4.9) gives;

$$O_a = 2.0831 + 0.0008X_A + 0.064X_B - 0.042X_C \qquad (10)$$

Equation (10) is the developed model equation for estimation of adsorption rate of oil in a contaminated site using Wood C for remediation process/clean up. The adsorption rate equation established a function of sawdust dosage, weight of absorbent and concentration of oil waste effluent discharged into the environment. For the case of wood C. Equation (10) is applicable in monitoring and simulating the rate of adsorption oil in clean up system.

In the case of wood c, the relationship between experimental oil adsorbed and the validated modeled oil adsorbed were assessed using coefficient of determination of the best fit, evaluated as R^2 = 0.85. The value of coefficient of correlation obtained is as result of functional parameters substituted in the development of the mathematical model. Figure 3 shows an acceptable trend of behavior between the experimental oil adsorbed and validated modeled oil adsorbed against demonstrating the useful of the developed modeled for monitoring of adsorption rate of oil in a contaminant site using Wood type B in the predicting, monitoring and simulation of adsorbed oil in the process of oil remediation from a polluted environment.

WOOD D: development of model equation for Wood D that predict rate of adsorption of oil in remediation process for the case of Wood D, the applicable normal equation is of the form;

$$\begin{Bmatrix} 4 & 110 & 26.5 & 241.2 \\ 110 & 3900 & 931 & 6214 \\ 265 & 931 & 222.3 & 1498 \end{Bmatrix} \begin{Bmatrix} a_0 \\ a_1 \\ a_2 \end{Bmatrix} = \begin{Bmatrix} 3.7 \\ 1167 \\ 27.7 \end{Bmatrix} \qquad (11)$$

Solving Equation (11) by method of elimination for determining the values of a_0, a_1, a_2, a_3 yields;

$$\begin{Bmatrix} a_0 \\ a_1 \\ a_2 \end{Bmatrix} = \begin{Bmatrix} 0.6975 \\ 0.2938 \\ -1.1971 \end{Bmatrix} \qquad (12)$$

Putting Equation (12) into equation (1) gives;

$$O_a = 0.6975 + 0.2938X_A - 1.1971X_B + 0.0013X_C \qquad (13)$$

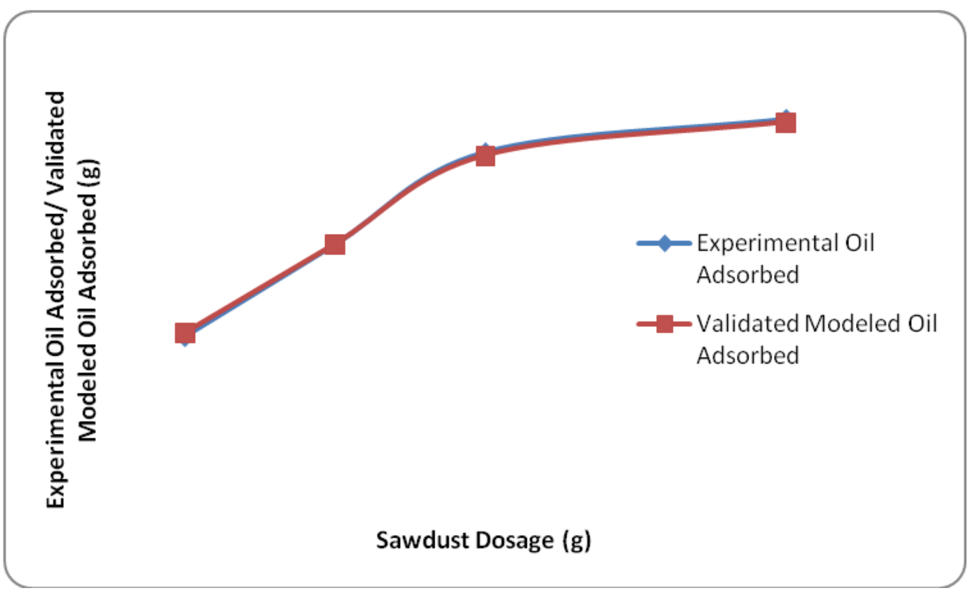

Figure 4 Plot of Experimental oil adsorbed and Validated modeled oil adsorbed versus Sawdust dosage

Equation (13) is the developed equation which can be used to monitor or simulate the rate of adsorption of oil using the case of wood D for the purpose of remediation of a polluted site. The relationship between the experimental and modeled adsorption rate of oil was evaluated by determining the coefficient of determination R^2 =1.0

Figure 4 shows the between the experimental oil adsorbed and validated modeled oil adsorbed versus dosage. The multiple regression model application in monitoring and simulating the rate of adsorption in cleaning a polluted site using the Wood D. The developed model performed very well in predicting the rate of adsorption of oil in this case.

Table 2 Summary of Developed Multiple Regression Model for Wood A, B, C and D

Wood Type	Trend of Developed Equation	Coefficient of Determination for validation, R^2
A	$1.0128+0.0055X_A+0.092X_B-0.0012X_C$	0.96
B	$-0105+0.0216X_A+0.0001X_B+0.0028X_C$	0.76
C	$2.0831+0.0008X_A+0.064X_B-0.042X_C$	0.85
D	$0.6975+0.2938X_A-1.1971X_B+0.0013X_C$	1.00

Models on Effect of Temperature on Oil Sorption Capacity (S_c)

In developing this model, the linear regression concept will be used. Since oil sorption capacity depends upon temperature.

$$S_c = a_0 + a_1T \qquad (14)$$

Where, S_c = oil sorption capacity, T= temperature a_0 and a_1 = constant coefficient of sorption capacity.

Equation (14) is used to develop a Mathematical Model in a form of a linear equation to investigate the variation of temperature and it results on oil sorption capacity values for all cases of the wood been used in this research assessment.

WOOD A: Developing a linear regression model that predict the effect of temperature on oil sorption normal equation generated is of the from**;**

$$\begin{Bmatrix} 4 & 120 \\ 120 & 4100 \end{Bmatrix} \begin{Bmatrix} a_0 \\ a_1 \end{Bmatrix} = \begin{Bmatrix} 250 \\ 7480 \end{Bmatrix} \qquad (15)$$

Solving Equation (15) by method of elimination gives;

$$\begin{Bmatrix} a_0 \\ a_1 \end{Bmatrix} = \begin{Bmatrix} 63.7 \\ -0.04 \end{Bmatrix} \qquad (16)$$

Putting equation (16) into equation (14) gives;

$$S_c = 63.7 - 0.047\ T \qquad (17)$$

Equation (17) is the simulating or monitoring equation developed to study the effect of variation temperature on oil sorption capacity

Table 3 Simulation of the effect of variation of temperature on oil sorption capacity Wood A

Temperature	**Experimental oil Sorption Capacity**	**Validation Modeled oil Sorption Capacity**
15	60.0	63.1
25	68.40	62.7
35	60.20	62.3
45	61.40	61.70

WOOD B. Developing a linear regression model that predict the effect of temperature on oil sorption capacity. Normal equation generated is of the form:

$$\begin{Bmatrix} 4 & 120 \\ 120 & 4100 \end{Bmatrix} \begin{Bmatrix} a_0 \\ a_1 \end{Bmatrix} = \begin{Bmatrix} 624 \\ 1854 \end{Bmatrix} \quad (18)$$

Solving equation (q) by method of matrix elimination gives;

$$\begin{Bmatrix} a_o \\ a_1 \end{Bmatrix} = \begin{Bmatrix} 16.68 \\ -0.036 \end{Bmatrix} \quad (19)$$

Substituting values of a_o and a_1 into equation (4, 19) yielded;

$$SC = 16.68 - 0.036T \quad (20)$$

Equation (20) can be used to monitor or simulate oil sorption capacity as temperature changes

Table 4 Experimental oil sorption capacity and validation modeled oil sorption for Wood B

Temp.	Experimental Oil Sorption Capacity	Validation modeled Oil Sorption capacity
15	14.2	16.14
25	19.2	15.78
35	14.5	15.42
45	14.5	15.06

Wood C: Model Development of effect of temperature on oil sorption capacity by approach of linear regression. For the case of wood C, the generated equation is of the form:

$$\begin{Bmatrix} 4 & 120 \\ 120 & 4100 \end{Bmatrix} \begin{Bmatrix} a_o \\ a_1 \end{Bmatrix} = \begin{Bmatrix} 296 \\ 8863 \end{Bmatrix} \quad (21)$$

Equation (21) were solved by approach of matrix elimination method and gives the result below;

$$\begin{Bmatrix} a_0 \\ a_1 \end{Bmatrix} = \begin{Bmatrix} 75 \\ -0.034 \end{Bmatrix} \quad (22)$$

putting equation (22) into equation (14) gives;

$$S_C = 75 - 0.034T \quad (23)$$

Equation (23) is the simulating or monitoring developed equation to study the effect variation of temperature on oil sorption capacity for wood type C.

Table 5 Simulation of the effect of variation of temperature on oil sorption capacity for Wood C

Temp.	Experimental Oil Sorption Capacity	Validation modeled Oil Sorption capacity
15	72.4	74.49
25	78.68	74.15

35	72.50	73.81
45	72.72	73.47

WOOD D: Developing a linear regression model that predicts the effect of temperature on oil sorption capacity. Normal equation generated is of the form:

$$\begin{Bmatrix} 4 & 120 \\ 120 & 4100 \end{Bmatrix} \begin{Bmatrix} a_0 \\ a_1 \end{Bmatrix} = \begin{Bmatrix} 166 \\ 4987 \end{Bmatrix} \qquad (24)$$

Solving equation (24) by method of matrix elimination gives;

$$\begin{Bmatrix} a_0 \\ a_1 \end{Bmatrix} = \begin{Bmatrix} 41.08 \\ 0.014 \end{Bmatrix} \qquad (25)$$

Substituting the values of a_0 and a_1 into equation (14) yielded;

$$S_C=41.08+0.014T \qquad (26)$$

Equation (26) is developed to monitor and simulate the effect of temperature on oil sorption capacity for wood type D.

Table 6 Simulation of the effect of variation of temperature on oil sorption capacity for Wood D

Temperature	Experimental oil sorption capacity	Validation modeled oil sorption capacity
15	40.60	41.29
25	43.80	41.43
35	41.02	41.57
45	41.25	41.71

CONCLUSION

The following conclusion can be drawn from the investigation as stated below:

1. Multiple regression technique is found useful in monitoring, predicting and simulating the rate crude oil adsorption in water and soil environment.
2. The application of the Regression approach was introduced to examine the effect of temperature on the rate of adsorption process during remediation of crude oil polluted site environment.
3. The approach adopted during this research work revealed that the multiple regression process is found useful in the determination of coefficient and the functional parameters that controls the rate of adsorption of crude oil upon dependents of the degree of the dosage.
4. The research work demonstrates the significance of the wood sawdust characteristics on the rate of crude oil adsorption in the process reactor.
5. It is observed that the weight of the wood sawdust is a contributing factor to the rate of adsorption of crude oil in the process reactor.

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